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Exploring the Interdependencies Between Parameters in a Material Model

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Abstract

A method is investigated to reduce the number of numerical parameters in a material model for a solid. The basis of the method is to detect interdependencies between parameters within a class of materials of interest. The method is demonstrated for a set of material property data for iron and steel using the Johnson-Cook plasticity model.

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Contents

1 Introduction

Many material models for use in modern simulation software have a large number of material dependent parameters. A large number of parameters causes difficulty for at least four reasons:

- It can be time consuming and expensive to design and conduct experiments to explicitly determine all the necessary parameters for a given material.
- To investigate changes to a measurable material property such as yield stress might require changes to multiple parameters in the model, because of possible interdependence between them.
- When undertaking a material optimization or sensitivity study, it becomes time consuming to apply the necessary statistical variations to a large number of input parameters.
- Such an optimization study might give misleading results if material parameters are falsely assumed to be independent of each other, leading to an optimized material that cannot be obtained in real life.

It is therefore desirable to investigate ways of reducing the number of material parameters. In general, it is not satisfactory to simply assume that one or more parameters is constant, because in reality, it may not be possible to fabricate real materials with arbitrarily chosen parameters. For example, suppose an aerospace company wishes to explore the effect of using alternative types of composite materials for an aircraft design. The available material model predicts the stress tensor $\boldsymbol{\sigma}$ as a function of the strain tensor $\boldsymbol{\epsilon}$. The model has two material parameters: elastic modulus E and mass density ρ. Thus, the model has the form

$$\boldsymbol{\sigma}(\boldsymbol{\epsilon}; E, \rho).$$

Suppose the material parameters are known to fall within the following limits for all real materials:

$$100\text{GPa} \leq E \leq 200\text{GPa}, \qquad 1500\text{kg/m}^3 \leq \rho \leq 2500\text{kg/m}^3,$$

providing a constraint on the parameters. But these limits do not provide *enough* constraint on the material parameters, because in real life (we suppose for purposes of explanation) stiffer composites always have higher density. Then there must exist some relation $E(\rho)$ that expresses this interdependence. Once this interdependence is known, we can write

$$\boldsymbol{\sigma}(\epsilon; \rho) = \boldsymbol{\sigma}(\boldsymbol{\epsilon}; E(\rho), \rho).$$

Thus, the original two-parameter model has become a one-parameter model. The present study proposes a statistical approach to detecting the interdependence between material parameters for a set of materials, such as the function $E(\rho)$.

2 Multiple linear regression

In this section we summarize the technique of *multiple linear regression*, a standard statistical technique for determining the interdependence between variables. Suppose there is a given sample of N numbers y_j, $j = 1, 2, \ldots, N$. Associated with each y_j is a set of M numbers x_{ij}, $i = 1, 2, \ldots, M$. Regression attempts to find M *regression coefficients* $b_1, b_2, \ldots, b_M$ such that the function defined by

$$\hat{y}(x_1, x_2, \ldots, x_M) = b_1 x_1 + b_2 x_2 + \cdots + b_M x_M$$

minimizes the error defined by

$$\epsilon = \sum_{j=1}^{N} \left(\hat{y}(x_{1j}, x_{2j}, \ldots, x_{Mj}) - y_j \right)^2.$$

After minimizing the error with respect to each b_i according to a standard method [1], the regression coefficients are found to be

$$\mathbf{B} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y},$$

where

$$\mathbf{B} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_M \end{bmatrix}, \qquad \mathbf{Y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}, \qquad \mathbf{X} = \begin{bmatrix} x_{11} & x_{21} & \ldots & x_{M1} \\ x_{12} & x_{22} & \ldots & x_{M2} \\ \vdots & \vdots & & \vdots \\ x_{1N} & x_{2N} & \ldots & x_{MN} \end{bmatrix}.$$

3 Interdependence between groups of parameters

Suppose a given material model has P parameters:

$$p_1, p_2, \ldots, p_P.$$

We attempt to find a mathematical relation between these parameters based on experimental data on some class of real materials. Assume that all P parameters are known for a set of N materials, whether from published test data or new tests. This set of materials and their parameters will be called the *sample*. The particular values of the parameters in the sample for material j are denoted by

$$p_{1j}, p_{2j}, \ldots, p_{Pj}.$$

To apply regression, the parameters are assembled into groups $G_1, G_2, \ldots, G_{M+1}$, where $M \geq 1$. Each group is a function of the P parameters:

$$\begin{aligned} G_1 &= \hat{G}_1(p_1, p_2, \ldots, p_P), \\ G_2 &= \hat{G}_2(p_1, p_2, \ldots, p_P), \\ &\vdots \\ G_{M+1} &= \hat{G}_{M+1}(p_1, p_2, \ldots, p_P). \end{aligned}$$

It is not necessary for the groups to be nondimensional. The $\hat{G}$'s can be nonlinear functions. For material j in the sample, the values of the groups are denoted

$$G_{1j}, G_{2j}, \ldots, G_{(M+1)j}.$$

Thus, for any j, $1 \leq j \leq N$,

$$G_{ij} = \hat{G}_i(p_{1j}, p_{2j}, \ldots, p_{3j}).$$

Now approximate a particular group, say G_{M+1}, in terms of the other groups. This is accomplished by using multiple linear regression to find a set of coefficients $b_1, b_2, \ldots, b_M$ such that

$$G_{M+1} = b_1 G_1 + b_2 G_2 + \cdots + b_M G_M. \tag{1}$$

According to the method discussed in Section 2, the regression coefficients are found from

$$\mathbf{B} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y}, \tag{2}$$

where

$$\mathbf{B} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_M \end{bmatrix}, \qquad \mathbf{Y} = \begin{bmatrix} G_{(M+1)1} \\ G_{(M+1)2} \\ \vdots \\ G_{(M+1)N} \end{bmatrix}, \qquad \mathbf{X} = \begin{bmatrix} G_{11} & G_{21} & \ldots & G_{M1} \\ G_{12} & G_{22} & \ldots & G_{M2} \\ \vdots & \vdots & & \vdots \\ G_{1N} & G_{2N} & \ldots & G_{MN} \end{bmatrix}.$$

It is assumed that a solution $\mathbf{B}$ to (2) can be found, that is, $\mathbf{X}^T\mathbf{X}$ is nonsingular. Using the resulting b_i values, (1) provides a relation between the material groups.

This procedure started with a model that has P parameters, all of which were apparently unrelated and capable of being varied independently. Based on the sample of experimental data for some class of real materials, the procedure arrived at a mathematical relation (1) between the parameters. This, in principle, amounts to eliminating one of the parameters, say p_e, $1 \leq e \leq P$, from the material model.

In general, the dependence between p_e and the remaining $P - 1$ parameters is implicit, because the G's in (1) could be nonlinear functions of the material parameters. However, a major simplification results if this parameter p_e appears in only one group. By suitable numbering of the groups, we can label group $M + 1$. In this case, p_e appears only in the left-hand side of (1), so, unless the form of G_{M+1} is complicated, p_e can be explicitly solved for in terms of the other parameters.

4 Example: Johnson-Cook steel parameters

The Johnson-Cook plasticity model [2] is a widely used model for the flow stress σ of a material in terms of the equivalent plastic strain ε, its time derivative $\dot{\varepsilon}$, and the temperature T. The form of the model is

$$\sigma = (A + B\varepsilon^n)(1 + C \log \dot{\varepsilon})(1 - T_h^m)$$

where A, B, C, m, and n are material parameters. T_h is the homologous temperature, defined by

$$T_h = \frac{T - T_{room}}{T_{melt} - T_{room}}$$

where T_{room} and T_{melt} are the room temperature and the melt temperature, respectively. Thus, the Johnson-Cook plasticity model has six material parameters: A, B, C, m, n, and T_{melt}.

The Johnson-Cook fracture model [3] provides a similarly structured model for failure strain ε_f. This is implemented in a simulation code through the failure criterion

$$\int_0^t \frac{\dot{\varepsilon}}{\varepsilon_f}\, dt \geq 1.$$

When the plastic strain at a point in the body accumulates to the extent that this inequality holds, fracture occurs. The expression for ε_f is

$$\varepsilon_f = \left(D_1 + D_2 e^{D_3 \sigma^*}\right)\left(1 + D_4 \log \dot{\varepsilon}\right)\left(1 + D_5 T_h\right)$$

where D_1, D_2, D_3, D_4, and D_5 are material parameters. σ^* is a measure of the hydrostatic stress relative to the deviatoric stress, defined by

$$\sigma^* = \frac{\sigma_{11} + \sigma_{22} + \sigma_{33}}{3Y}$$

where Y is the von Mises equivalent stress. In both the Johnson-Cook plasticity and fracture models, treatment of terms involving $\log \dot{\varepsilon}$ for small values of $\dot{\varepsilon}$ is left to the discretion of those who implement the models in simulation codes.

In the present study, we do not consider all the D's in the fracture model explicitly as material parameters. Instead, for purposes of illustration, only the uniaxial tensile strain at failure e_f is considered, neglecting the strain rate term and the temperature term in the fracture model. This is defined by

$$e_f = D_1 + D_2 e^{D_3/3}.$$

As an example of the technique described in the previous sections, we investigate interdependence between the following parameters: A, B, C, n, and e_f.

The study is restricted to iron and steel. A literature search turned up 29 sets of Johnson-Cook plasticity parameters for this class of materials. Of these, 17 additionally reported the Johnson-Cook fracture parameters. The materials are as follows:

- Armco electrical iron [2]
- Carpenter electrical iron [2]
- 1006 steel [2]
- 4340 steel [2]
- S7 tool steel [2]
- Steel A [4]
- Steel B [4]
- Steel C [4]
- Steel D [4]
- 4340 tempered martensite [4]
- RHA [4]
- 2in RHA [4]
- Weldox 460E (set 1) [5]
- 4142 steel [6]
- 1045 steel [7]
- DP600 dual phase steel (sheet) [8]
- DP600 dual phase steel (tube) [8]
- XC48 steel (AISI1048) [9]
- 1080 steel [10]
- VascoMax steel [10]
- 35NCD16 steel [11]
- 316L stainless steel [11]
- 42CD4U steel [11]
- S300 steel [11]
- Mild steel [12]
- DP590 steel [12]
- Weldox 460E steel (set 2) [13]

- Weldox 700E steel [13]
- Weldox 900E steel [13]

The materials listed as "Steel A," etc., have parameters that are export controlled and so are not identified in this document.

4.1 Case 1: relate B to A and n

This case attempts to determine a dependence of B on combinations of A and n within the sample of iron and steel alloys. The groups, which were arrived at through trial and error, are as follows:

$$\begin{aligned} G_1 &= 1 \\ G_2 &= A \\ G_3 &= A^4 \\ G_4 &= n^2 \\ G_5 &= n^2/A \\ G_6 &= A/B \end{aligned}$$

Note that G_6 is the only group that involves B, so we approximate this group by a linear combination of the other groups. Using the method described in the previous section, regression analysis was carried out to determine the coefficients $b_1^{(1)}$, $b_2^{(1)}$, $b_3^{(1)}$, $b_4^{(1)}$, and $b_5^{(1)}$ in the relation

$$G_6 = b_1^{(1)} G_1 + b_2^{(1)} G_2 + b_3^{(1)} G_3 + b_4^{(1)} G_4 + b_5^{(1)} G_5.$$

The results of fitting the coefficients to the material data with $N = 29$ and $M = 6$, using SI units, resulted in the following values:

$$\begin{aligned} b_1^{(1)} &= -3.9309 \times 10^{-01} \\ b_2^{(1)} &= 2.8495 \times 10^{-09} \\ b_3^{(1)} &= -2.0452 \times 10^{-37} \\ b_4^{(1)} &= -1.2104 \times 10^{+00} \\ b_5^{(1)} &= 4.9056 \times 10^{+08} \end{aligned}$$

The regression fit is shown in Figure 1. In this plot, the horizontal coordinate represents sample data for G_6. That is, for the dot in the figure representing material j in the sample,

the horizontal coordinate is G_{6j}, as determined from the sample data. The vertical axis represents values determined by the regression fit. For material j, the vertical coordinate is

$$b_1^{(1)} G_{1j} + b_2^{(1)} G_{2j} + b_3^{(1)} G_{3j} + b_4^{(1)} G_{4j} + b_5^{(1)} G_{5j}$$

where the values for $\{G_{1j}, G_{2j}, G_{3j}, G_{3j}, G_{4j}\}$ (but not G_{6j}) are taken from the sample data. The dashed line with slope 1 is shown for reference. If the regression fit were perfect, all the dots would fall on this line.

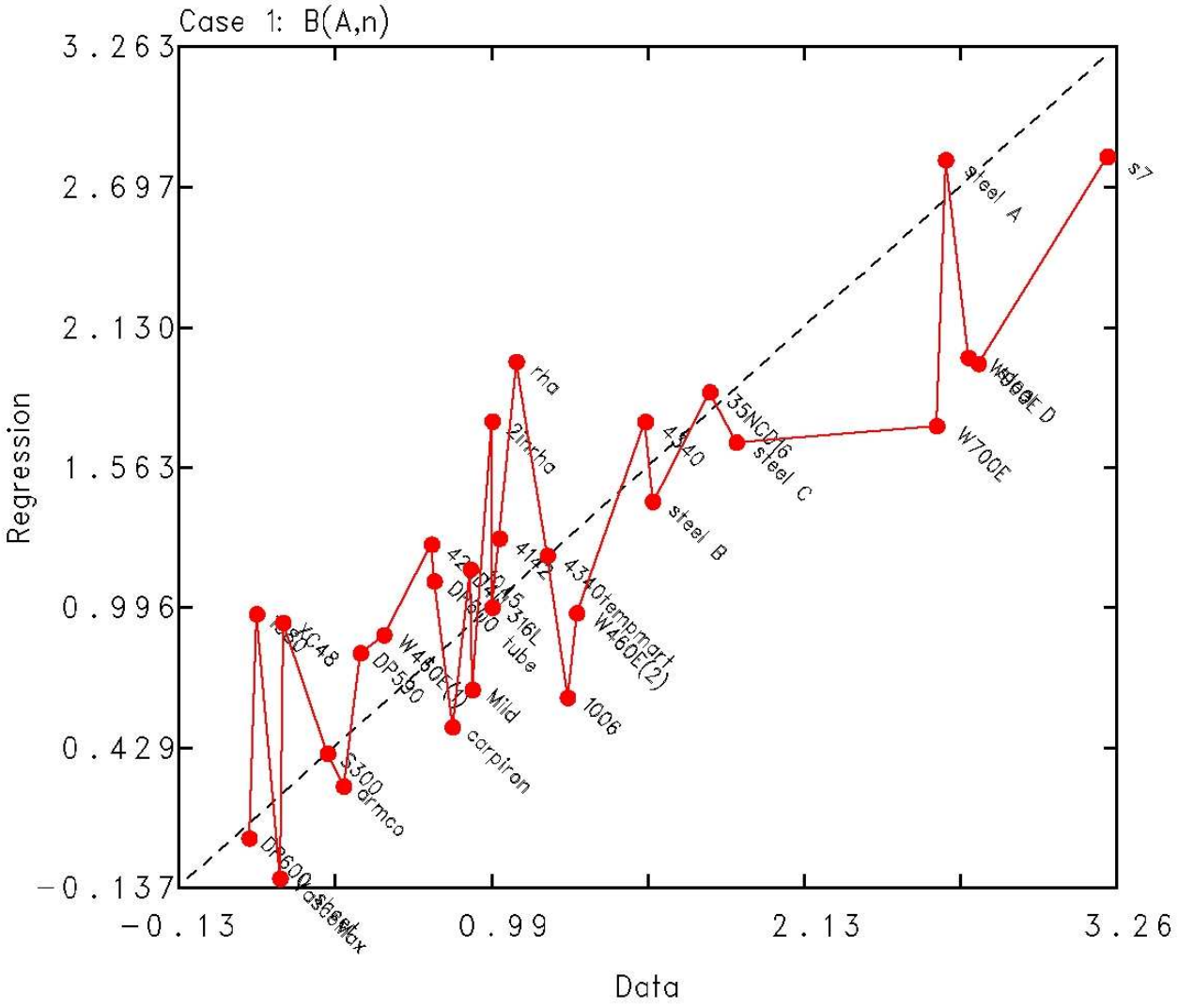

Figure 1. Regression fit for G_6 as a function of sample data in Case 1.

4.2 Case 2: relate C to A and B

This case attempts to determine a dependence of C on combinations of A and B. The groups, which were arrived at through trial and error, are as follows:

$$\begin{aligned} G_1 &= 1 \\ G_2 &= 1/\sqrt{A} \\ G_3 &= A/B \\ G_4 &= 1/A^2 \\ G_5 &= \sqrt{C} \end{aligned}$$

The coefficients in the regression fit for

$$G_5 = b_1^{(2)} G_1 + b_2^{(2)} G_2 + b_3^{(2)} G_3 + b_4^{(2)} G_4$$

ae found to be

$$\begin{aligned} b_1^{(2)} &= 2.5406 \times 10^{-01} \\ b_2^{(2)} &= -4.1232 \times 10^{-06} \\ b_3^{(2)} &= -9.8688 \times 10^{-03} \\ b_4^{(2)} &= 2.2887 \times 10^{+15}. \end{aligned}$$

The regression fit is shown in Figure 2.

4.3 Case 3: relate e_f to A, B, and n

This case attempts to determine a dependence of e_f on combinations of A, B, and n. The groups, which were arrived at through trial and error, are as follows:

$$\begin{aligned} G_1 &= 1 \\ G_2 &= ne^{-n} \\ G_3 &= 1/n^2 A \\ G_4 &= 1/(A + nB) \\ G_5 &= e_f. \end{aligned}$$

Because tabulated Johnson-Cook failure parameters are available for only 17 materials in the sample of 29, in this case $N = 17$. The coefficients in the regression fit for

$$G_5 = b_1^{(3)} G_1 + b_2^{(3)} G_2 + b_3^{(3)} G_3 + b_4^{(3)} G_4$$

ae found to be

$$\begin{aligned} b_1^{(3)} &= -8.2062 \times 10^{-01} \\ b_2^{(3)} &= 5.4919 \times 10^{+00} \\ b_3^{(3)} &= 1.1278 \times 10^{+07} \\ b_4^{(3)} &= 4.2377 \times 10^{+08}. \end{aligned}$$

The regression fit is shown in Figure 3.

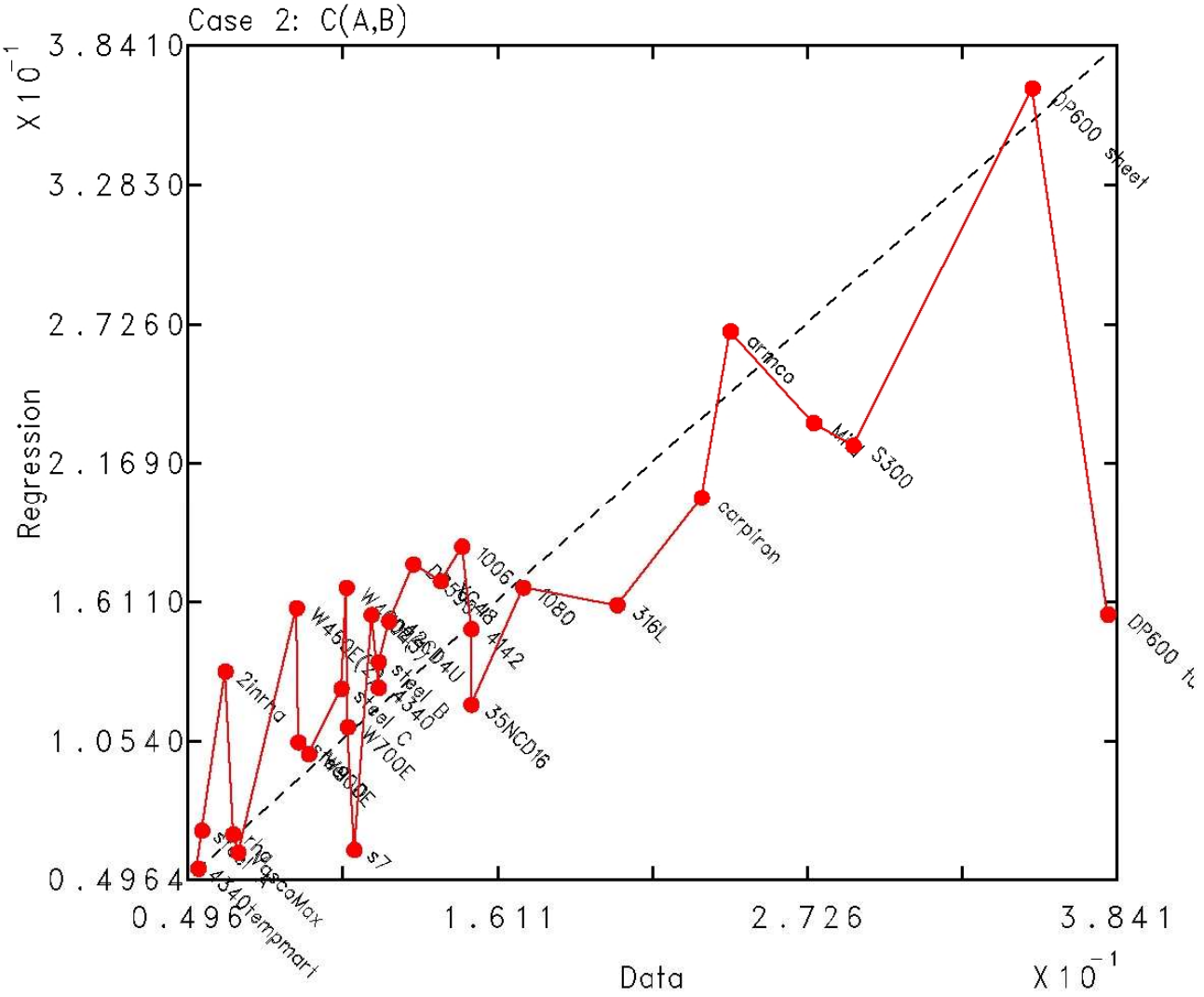

Figure 2. Regression fit for G_5 as a function of sample data in Case 2.

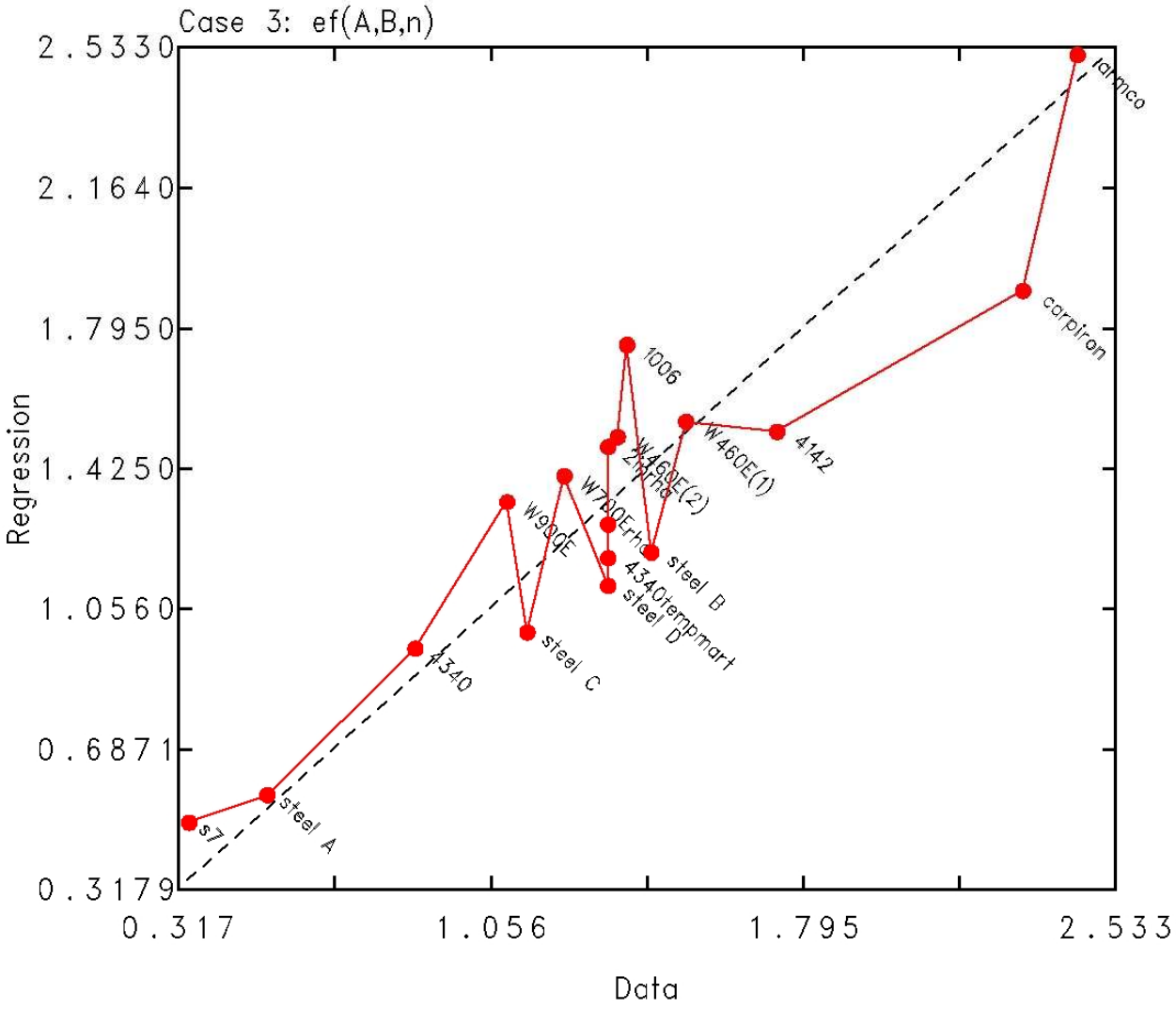

Figure 3. Regression fit for G_5 as a function of sample data in Case 3.

5 Discussion

The examples illustrate how the interdependencies between parameters within a class of materials (iron and steel) can be exploited to express one or more parameters in terms of the others, thus reducing the number of parameters in the model. In Case 1, the following relation was found:

$$\frac{A}{B} = b_1^{(1)} + b_2^{(1)} A + b_3^{(1)} A^4 + b_4^{(1)} n^2 + b_5^{(1)} \frac{n^2}{A},$$

which in effect eliminates B as an independent model parameter. From Case 2,

$$\sqrt{C} = b_1^{(2)} + b_2^{(2)} \frac{1}{\sqrt{A}} + b_3^{(2)} \frac{A}{B} + b_4^{(2)} \frac{1}{A^2},$$

which in effect eliminates C as an independent model parameter. From Case 3,

$$e_f = b_1^{(3)} + b_2^{(3)} n e^{-n} + b_3^{(3)} \frac{1}{n^2 A} + b_4^{(3)} \frac{1}{A + nB},$$

which predicts the failure strain in uniaxial tension.

The examples analyzing the Johnson-Cook parameters for iron and steel illustrate some results that are perhaps unexpected:

- Case 1 shows that B is correlated with A and n, a result that would probably not suggest itself from casual examination of the raw material test data.
- Case 2 shows that the constant in the *rate-dependent* term, C is related to the *static* parameters A and B.
- Case 3 shows that the failure strain in uniaxial tension, e_f, is related to the plasticity parameters A, B, and n. This result is not very surprising, because in real materials there is a well-known trade-off between flow stress and ductility.

Of course, the acceptability in applications of treating B, C, and e_f as dependent parameters is conditional on the acceptability of the regression fits, as illustrated in the figures. The material parameters in the iron and steel sample are derived from a number of different material testing techniques, and it is possible that if all the materials used exactly the same techniques, the regression fit might be tighter. No effort was made in this study to exclude any sets of parameters on the basis of quality of the data or testing methods. Also, the sample of 29 sets of material parameters included a spectrum of alloys with different compositions and processing techniques. In view of this, it is perhaps surprising that the trends shown in the examples are as strong as they are.

The groups $G_1, \ldots$ in most cases have no physical significance; they are merely combinations of parameters that result in a good fit when related to each other by linear regression. It should also be noted that dimensions and units have no importance in this analysis, as

long as a consistent set of units is used throughout. The regression coefficients b_i can have different dimensions from each other.

The primary disadvantage of the approach presented in this paper is that there is no automated way of defining the groups. At present, this can only be accomplished by trial and error, although this process can be informed by expected interdependencies based on physical insight. However, it seems possible that in the future, some method could be developed for identifying the groups that result in the best regression fit.

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